LA-UR-22-24252

Approved for public release; distribution is unlimited.

Title:	Materials Data Management at LANL and across the Nuclear Security Enterprise
Author(s):	Schembri, Philip Edward Hughey, Lisa Michelle O'Neel, Jillian Cathleen
Intended for:	For distributing slides after presentation to NNSA.
Issued:	2022-05-06

Los Alamos NATIONAL LABORATORY

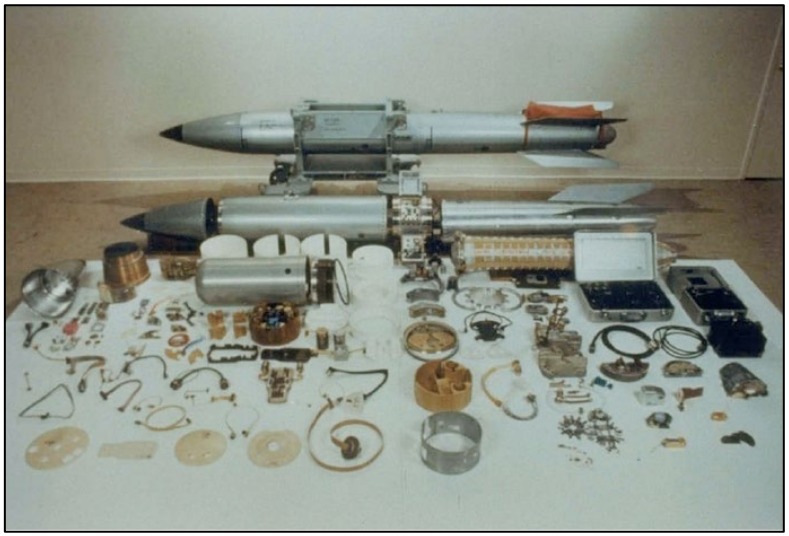
Materials Data Management at LANL and across the Nuclear Security Enterprise

Philip Schembri, Jillian O'Neel, Lisa Hughey

May 4, 2022

Agenda

- Why we need materials data management
- Materials data management at LANL
- Materials data management across the enterprise
- Critical gaps affecting enterprise deployment



- *Lots of parts…*
- *Lots of materials…*
- *Lots of data!*

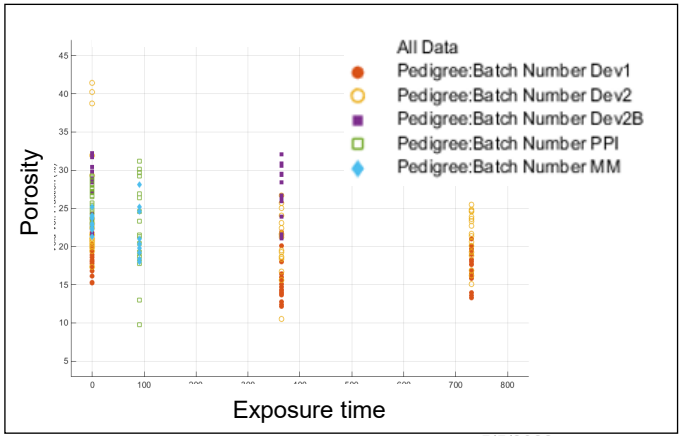
Why we need materials data management

Material data supports current and future nuclear deterrent

Common examples of materials data used in the weapons program:

- Material **compatibility** and aging tests
  - To prevent future SFNs/SFIs
- Material **model** calibration/validation
  - Engineering (simulating STS conditions)
  - Physics (simulating nuclear detonation)
- Weapons **design** and **product structure**
- Tracking materials **availability** issues
- Supporting material **development** & **replacement** efforts

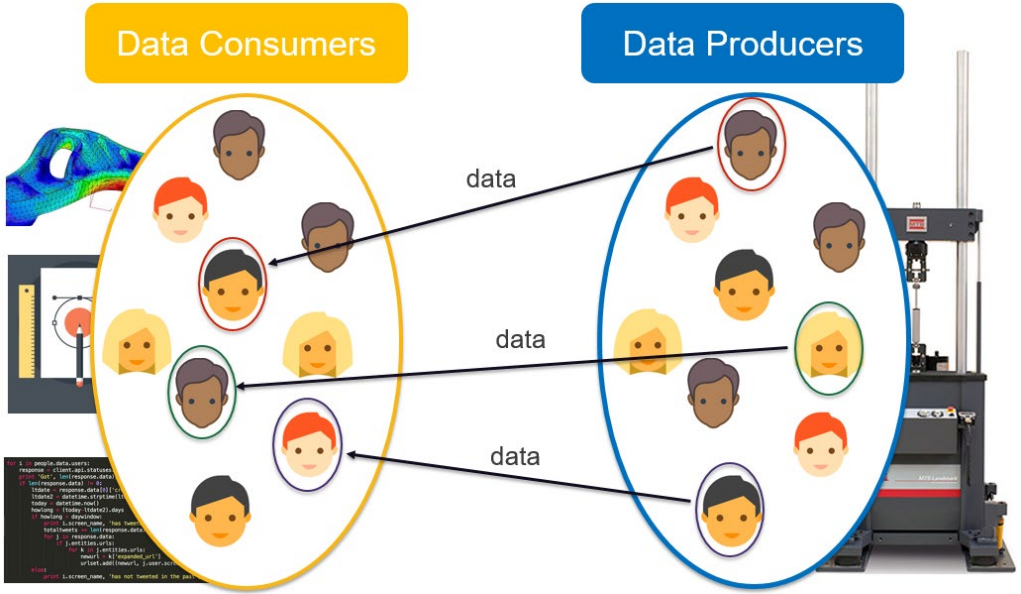
Dynamic deformation of materials



Porosity of replacement foam per batch

Materials data is lost without effective data management

- Test data is **valuable**
  - $0.5M to $40M per test series
  - Many test series each year
  - Some data is irreplaceable
- Previous ‘solutions’:
  - Data stored on **individual hard drives**
  - Data transferred via **email**
  - Local **experts** are ‘keepers of the data’
- Without materials data management:
  - **Data is lost**
  - Lost opportunity for data to inform future work
  - Lost opportunity to apply modern data analysis tools (e.g. machine learning)

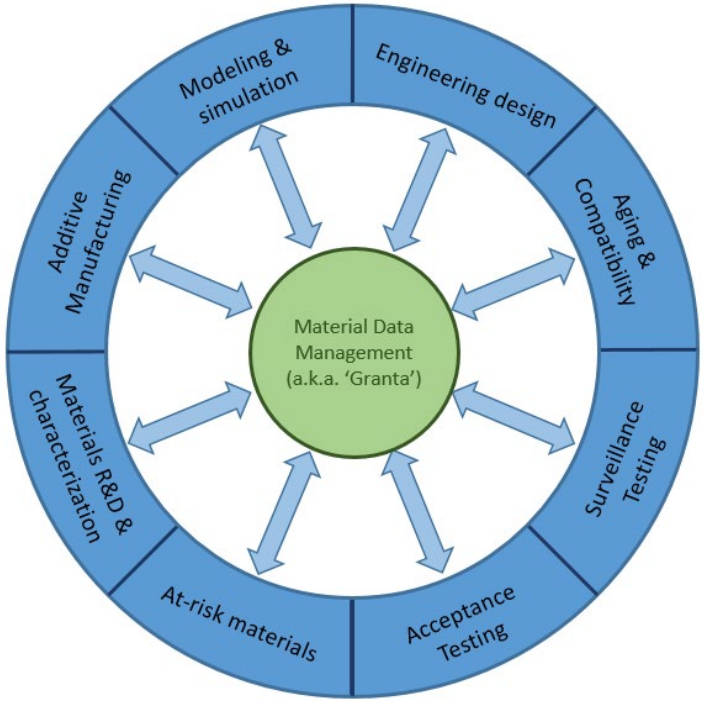


Data was transferred between individuals instead of being centrally available

Solution: ‘single source of truth’ for materials data

The solution was designed to include:

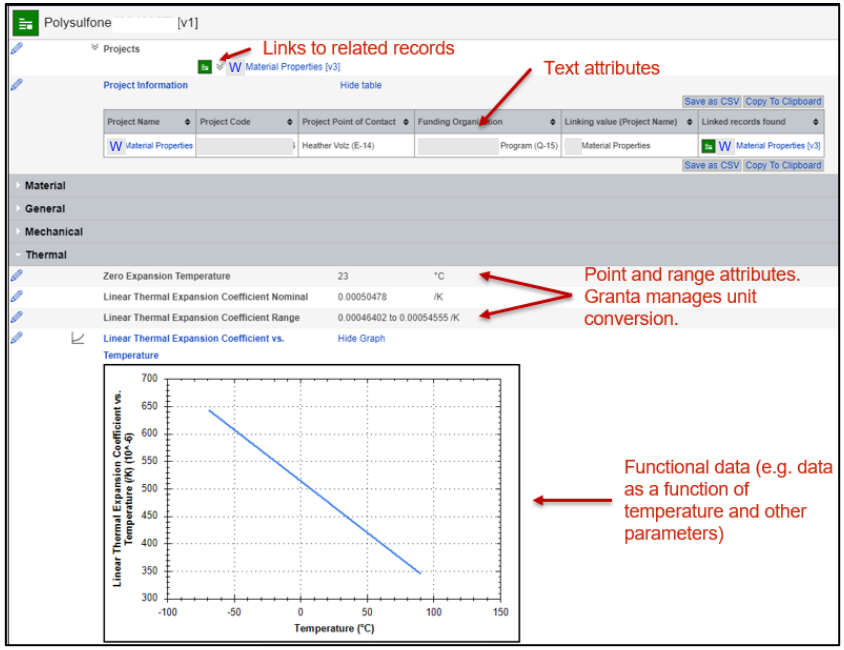
- Upload of legacy data
- Tools to upload new data at birth
- Accommodation of multiple types of data:
  - Test data (many types)
  - Images (micrographs, computed tomography)
  - Material properties
  - Material models
- Integration of data with:
  - PLM (PDMLink)
  - CAD (Creo)
  - Simulation (Abaqus, Sierra, MCNP, etc.)



LANL has made significant progress, enabled primarily by Archiving & Support

LANL uses Granta:MI software for materials data management

- Founded at Cambridge University (1994)
- Granta Design bought by **ANSYS** (2018)
- SQL technology:
  - Web **browser**-based
  - **Python** Software Toolkit & other APIs
- Industry standard:
  - Rolls-Royce, Boeing, NASA, Lockheed, etc
- Enterprise license contract for **all NSE sites** (courtesy of PRIDE; NA-122.1)

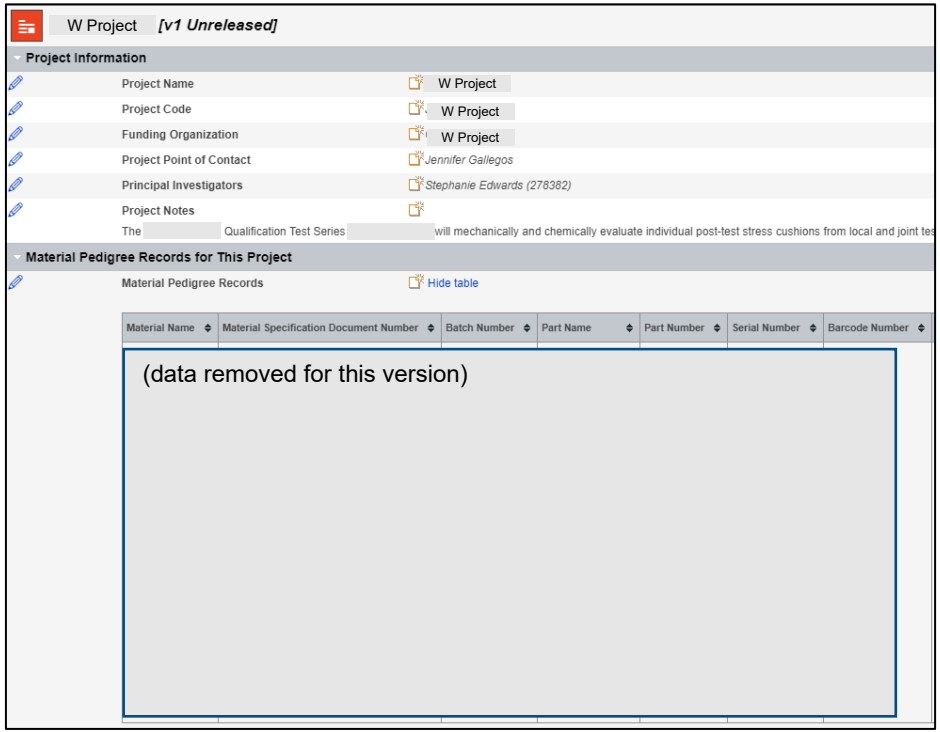


Primary access is browser-based

Materials data management at LANL

Example: Interrogating foam data supporting NA-125

- **Objective**: understand the effect of processing and environment on foam porosity



- Foam materials:
  - Help ensure ‘package’ is delivered intact
  - Do a very specific job
  - Must be precisely understood

- Many tests performed (MST-7)
- Data uploaded to Granta
- Tracked for each test specimen:
  - Batch
  - Part Name
  - Part Number
  - Serial Number
  - Environmental exposure time
  - Environmental exposure temperature

Example: Interrogating foam data supporting NA-125

- CT images (analyzed for void volume fraction) were uploaded to Granta

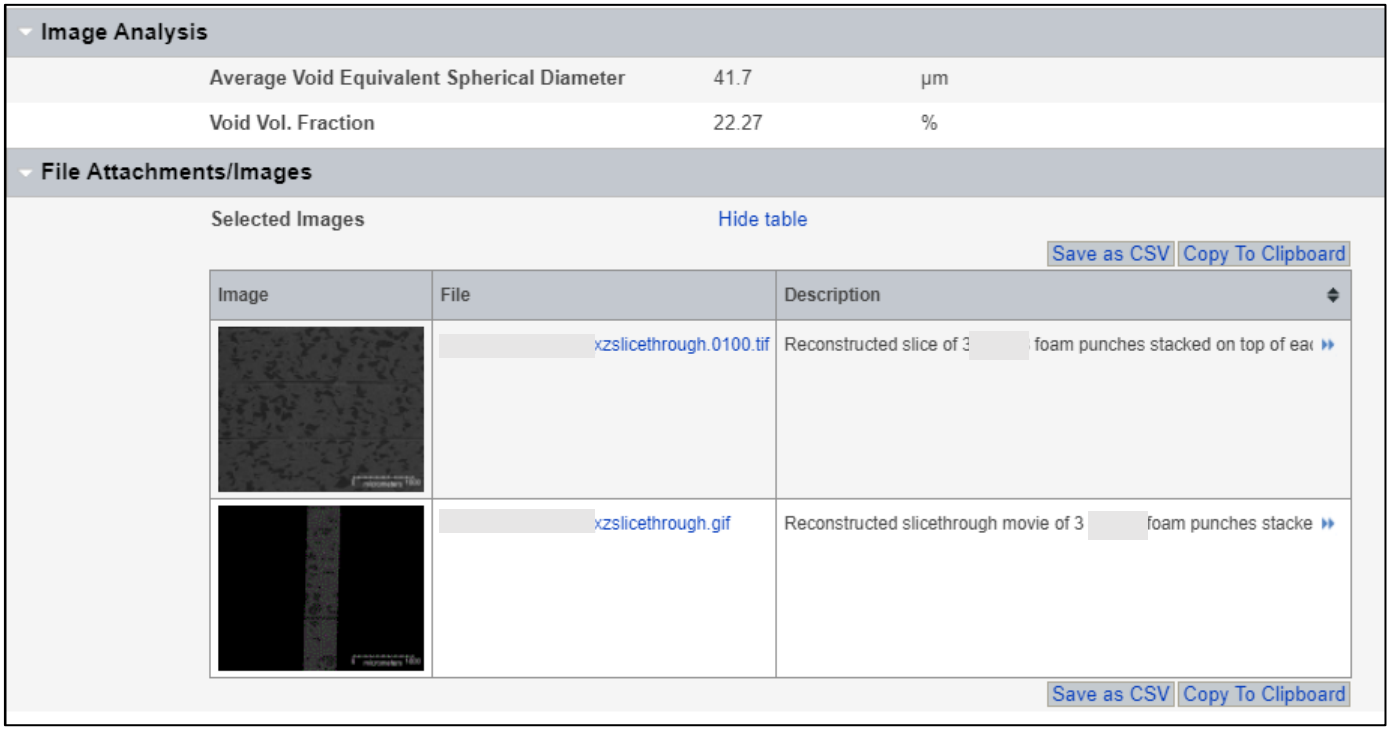


Image Analysis

Average Void Equivalent Spherical Diameter	41.7	µm
Void Vol. Fraction	22.27	%

File Attachments/Images

Selected Images — Hide table

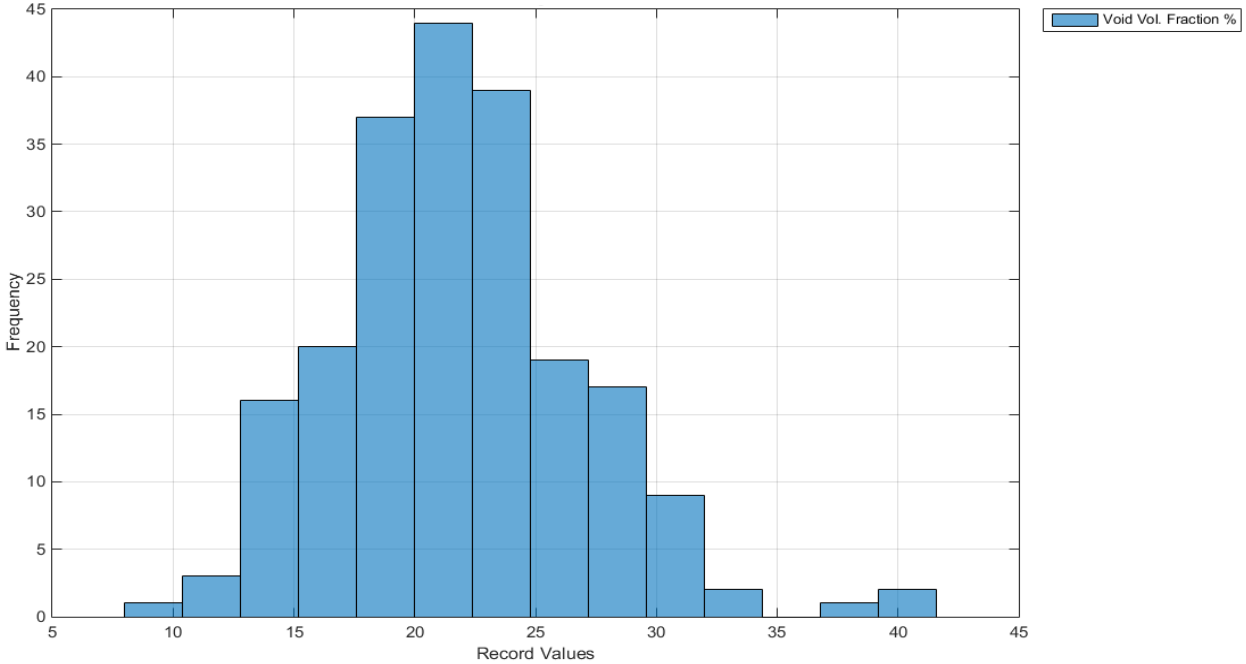
Save as CSV | Copy To Clipboard

Image	File	Description
	xzslicethrough.0100.tif	Reconstructed slice of 3 foam punches stacked on top of ea
	xzslicethrough.gif	Reconstructed slicethrough movie of 3 foam punches stacke

Save as CSV | Copy To Clipboard

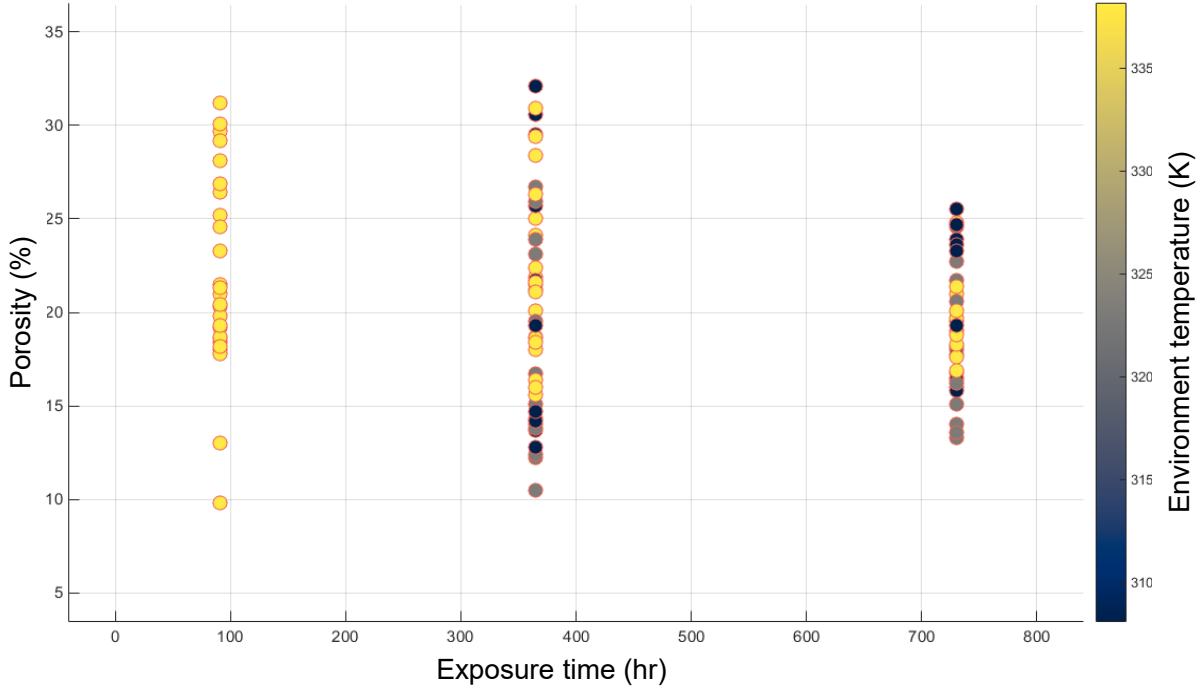
Example: Interrogating foam data supporting NA-125

- Granta:MI provides visualization tools
  - E.g. Histogram of void volume fraction



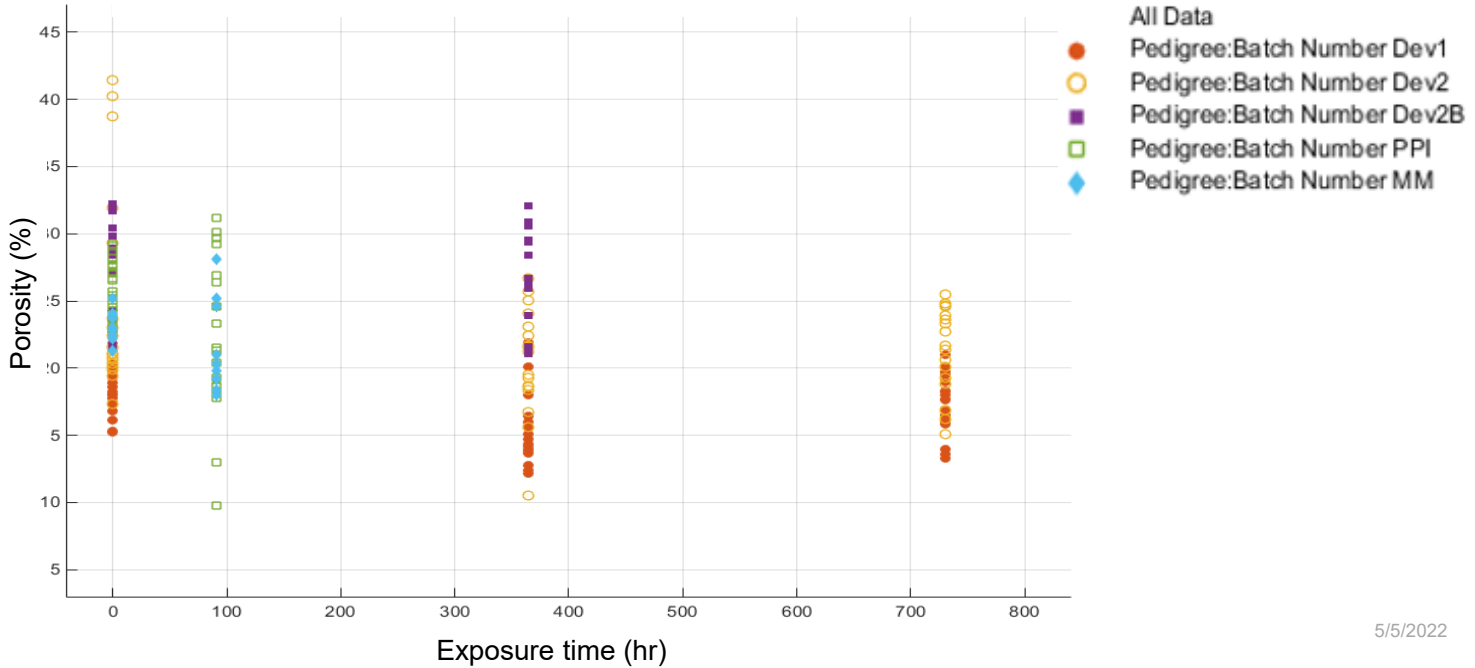
Example: Interrogating foam data supporting NA-125

- Granta:MI provides visualization tools
  - E.g. Effect of exposure time and temperature on void volume fraction



Example: Interrogating foam data supporting NA-125

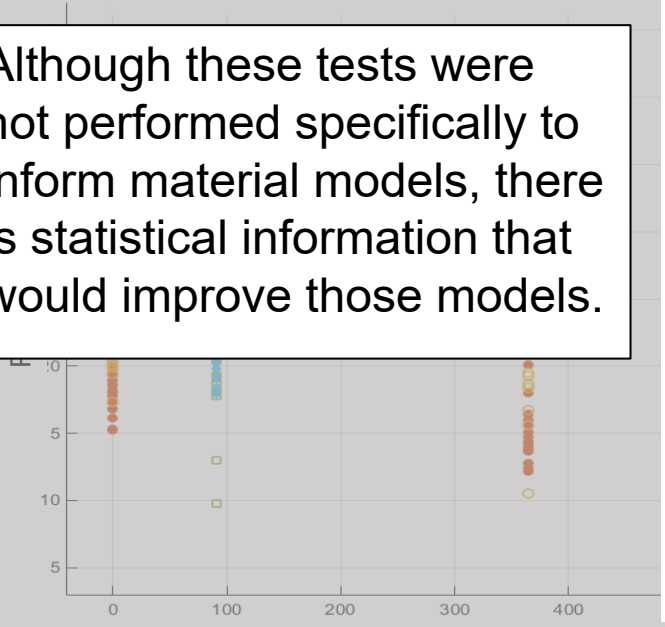
- Granta:MI provides visualization tools
  - E.g. Effect of exposure time and batch number on void volume fraction

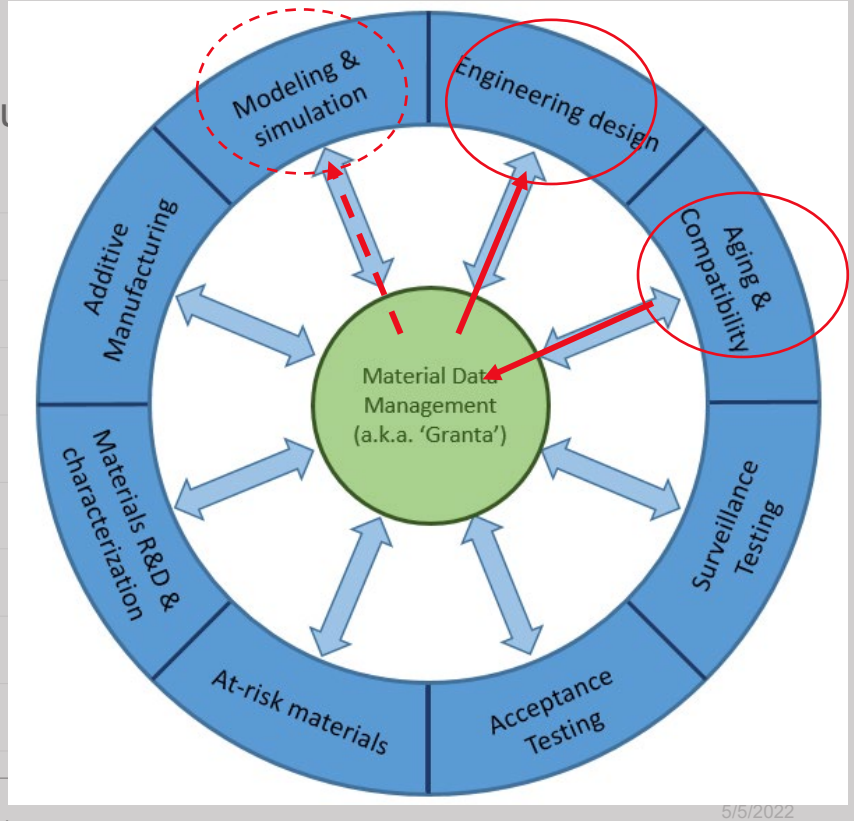


Example: Interrogating foam data supporting NA-125

- Granta:MI provides visualization tools
  - E.g. Effect of exposure time and batch nu

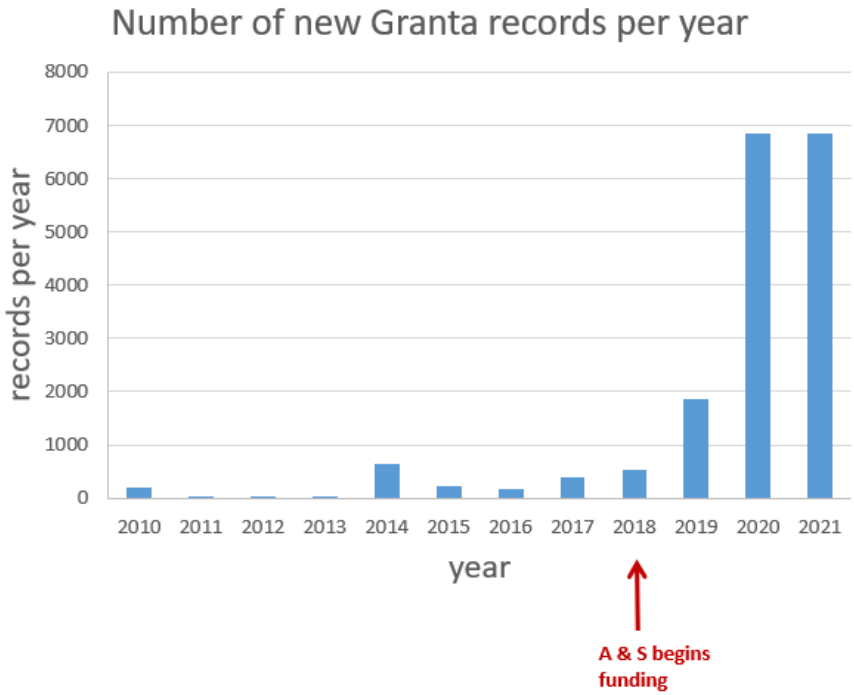
Although these tests were not performed specifically to inform material models, there is statistical information that would improve those models.





Granta:MI usage at LANL

- Total number of users = 250
- Data being uploaded:
  - Many materials: polymers, foams, metals
  - Mechanical tests – static and dynamic
  - Thermal and chemical tests
  - Images
  - Legacy and new data
  - Additive manufacturing (AM) parameters & performance
  - Documents
- Data being used for:
  - New design activities
  - Material model calibration
  - Additive manufacturing design

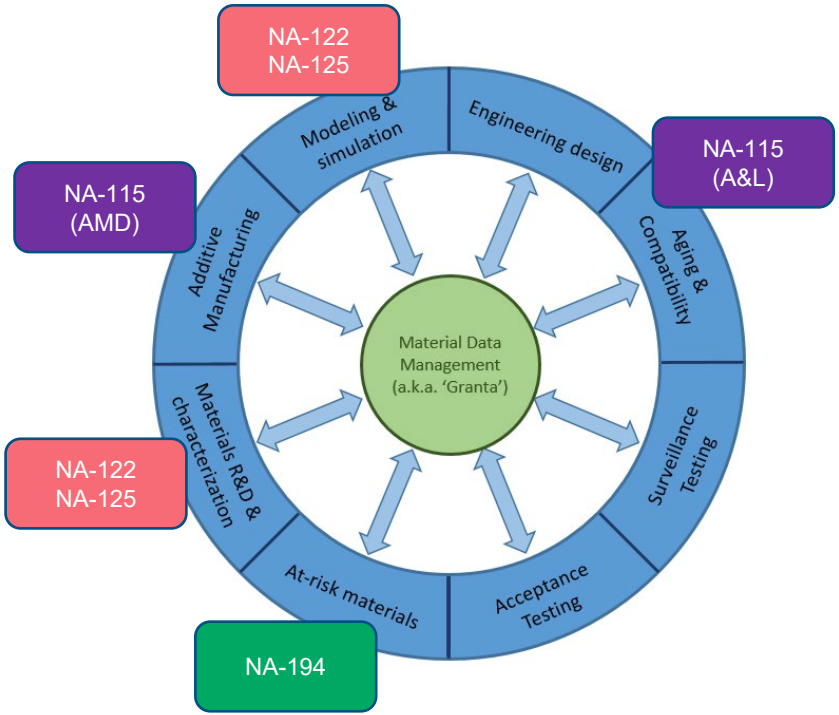


Many programs use and support Granta:MI

- PRIDE (NA-122.1)
  - Coordinates funding for licenses from other programs
  - Supports Operation & Maintenance (O&M) of NSE-wide Granta:MI instances

- Archiving and Support (NA-115):
  - Tool & process development for data upload
  - Upload of legacy data
  - Documentation

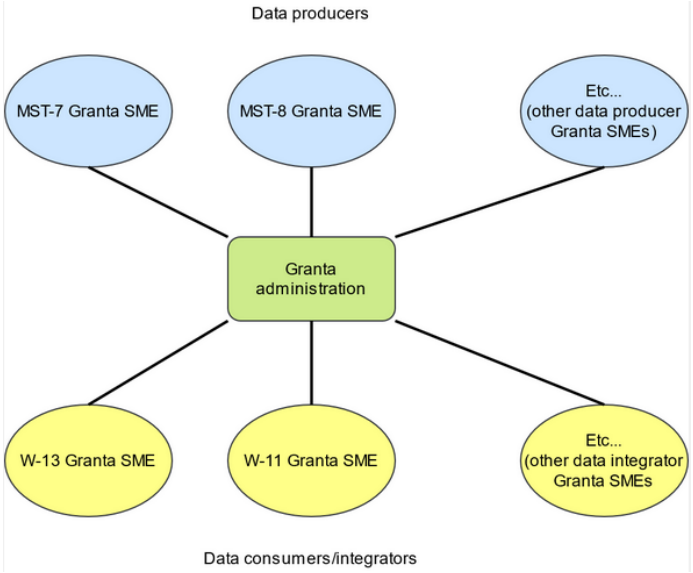
- Other projects/programs manage their data using Granta:MI
  - NA-122/125: Material characterization & modeling
  - NA-115 (AMD): Additive manufacturing
  - NA-115 (A&L): Aging and Lifetimes
  - NA-194: At-Risk Materials



Many programs make use of Granta:MI

Consistent A&S support enabled Granta:MI to be a LANL-wide resource

- **In the past**:
  - Granta:MI was managed/used by a few ‘champions’.
  - Development was ad-hoc; not very standardized
- **Now**: Consistent funding has enabled:
  - Establishing well-defined roles; e.g.:
    - To manage hardware/software
    - To manage data upload
  - Granta:MI to support the entire weapons program
  - Standardization and documentation



Granta:MI now supports the entire weapons program

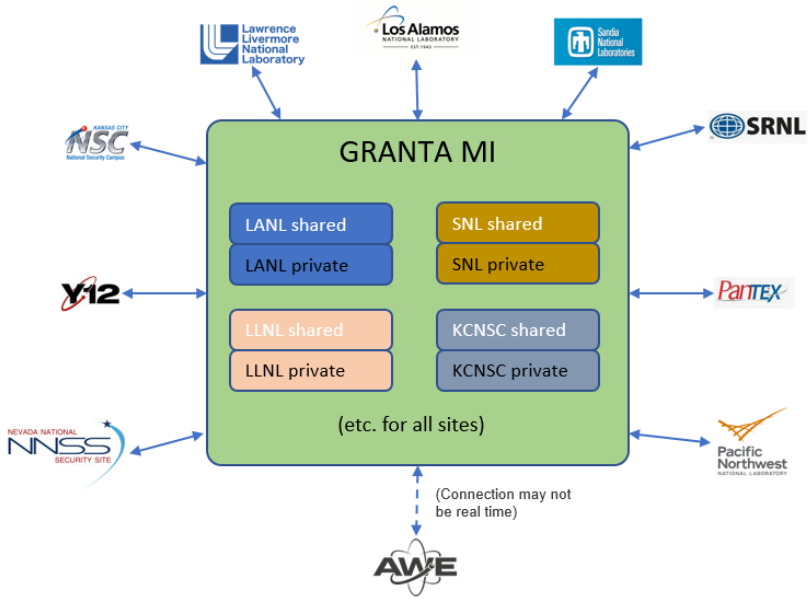
Materials data management across the enterprise

Other NSE sites also use Granta:MI and are going through the same process as LANL

- SNL & KCNSC: actively managing data with Granta:MI
- LLNL & SRNL: ramping up their implementations
- PX, Y-12, NNSS, PNNL: no local Granta:MI installation but recognize need
- Types of data at other sites include:
  - High Explosives (HE)
  - Acceptance and surveillance tests
  - Hydrogen embrittlement data
  - Other specialized materials

An enterprise Granta:MI instance is in limited use

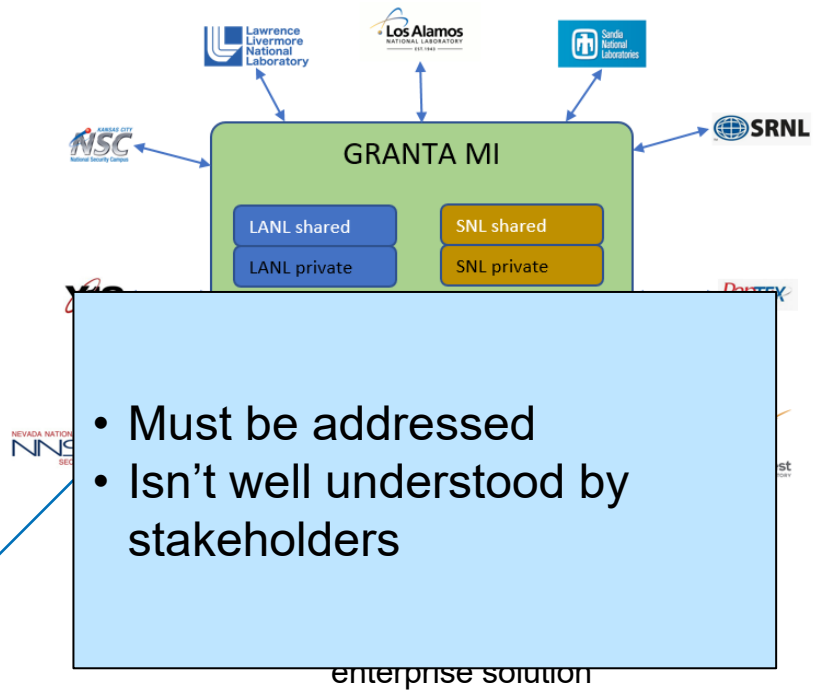
- Move towards **enterprise** Granta:MI instances to enable:
  - Cost savings (fewer servers)
  - Data sharing across sites
  - Common tools for upload/report
  - Engagement of other sites (PX, Y12, NNSS)
- LANL hosts ESN Granta:MI instance, funded by PRIDE
  - Used by **At-Risk Materials** (NA-194)
  - Strong push from NA-115 for AM projects
- Two major challenges:
  - **IT:** Network configuration, authentication, etc
  - **Data:** Standardizing database schema



Granta:MI is being implemented as an enterprise solution

An enterprise Granta:MI instance is in limited use

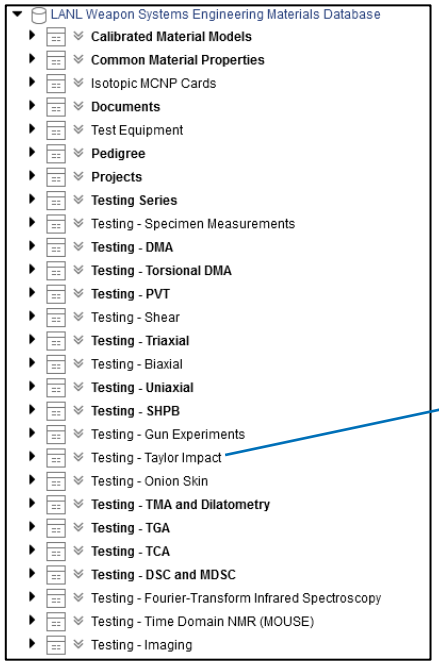
- Move towards **enterprise** Granta:MI instances to enable:
  - Cost savings (fewer servers)
  - Data sharing across sites
  - Common tools for upload/report
  - Engagement of other sites (PX, Y12, NNSS)
- LANL hosts ESN Granta:MI instance, funded by PRIDE
  - Used by **At-Risk Materials** (NA-194)
  - Strong push from NA-115 for AM projects
- Two major challenges:
  - **IT:** Network configuration, authentication, etc
  - **Data:** Standardizing database schema



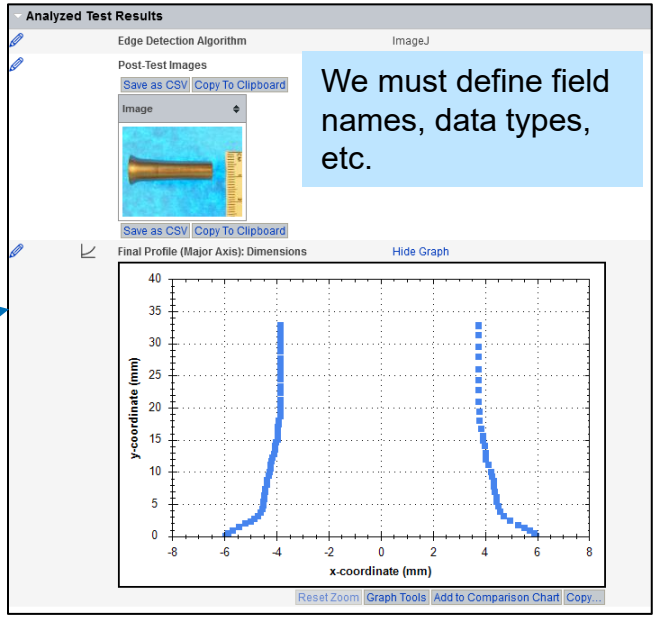
Critical gaps preventing enterprise deployment

Why standardizing schema is a challenge

- **Schema** = field names, types, definitions; data structure
- Granta:MI schema requires configuration



Granta doesn't know what a 'Taylor Impact Test' is… we have to tell it.



We must define field names, data types, etc.

Configuring Granta:MI takes significant effort

- Many decisions must be made:
  - Field names & definitions
    - Example: ‘Specimen’ vs. ‘Sample’, etc.
  - Data types
    - Text, pull-down menu, point, curve, etc
    - Choices affect ease of data upload, search and reporting
  - Database structure
    - Link data vs. duplicate data
  - Decisions must be discussed and documented
  - Consistency is critical
- There are many types of data
  - Material properties & models
  - Test data: *45 types of test identified*
  - Specifications
  - At-risk materials information
  - AM data
  - Etc…

Testing Type	Category	Priority	Priority	Priority	Priority	Priority	Priority	Priority	Priority	Pr
		SNL	KCNSC	LANL	PX	Y12	SRNL	PNNL	NA-193	NI
DSC	Thermal/chemical	3	2	3	3		3			
TGA	Thermal/chemical	3	2	3	3		3			
Particle size and shape	Powder characterization (?)	3	3	3	1		3			
Quasi-static uniaxial	Mechanical	3	3	3			3			
Corrosion	Thermal/chemical	3	3	3			3			
Surface roughness	Weight and dimensions	3	3	3			3			
Computed tomography	Imaging	3	3	3			3			
TMA	Thermal/chemical	3		3	3		2			
Powder flow	Powder characterization (?)	3	3	3			2			
FTIR	Spectroscopy	1	2	3	2		2			
Density	Weight and dimensions	3	3	2			2			
Gas gun	Mechanical	2	2	3			1			
Grain size analysis	Weight and dimensions (or Imaging?)	2	3	1			2			
NMR (Mouse)	Spectroscopy	1		1	3		2			

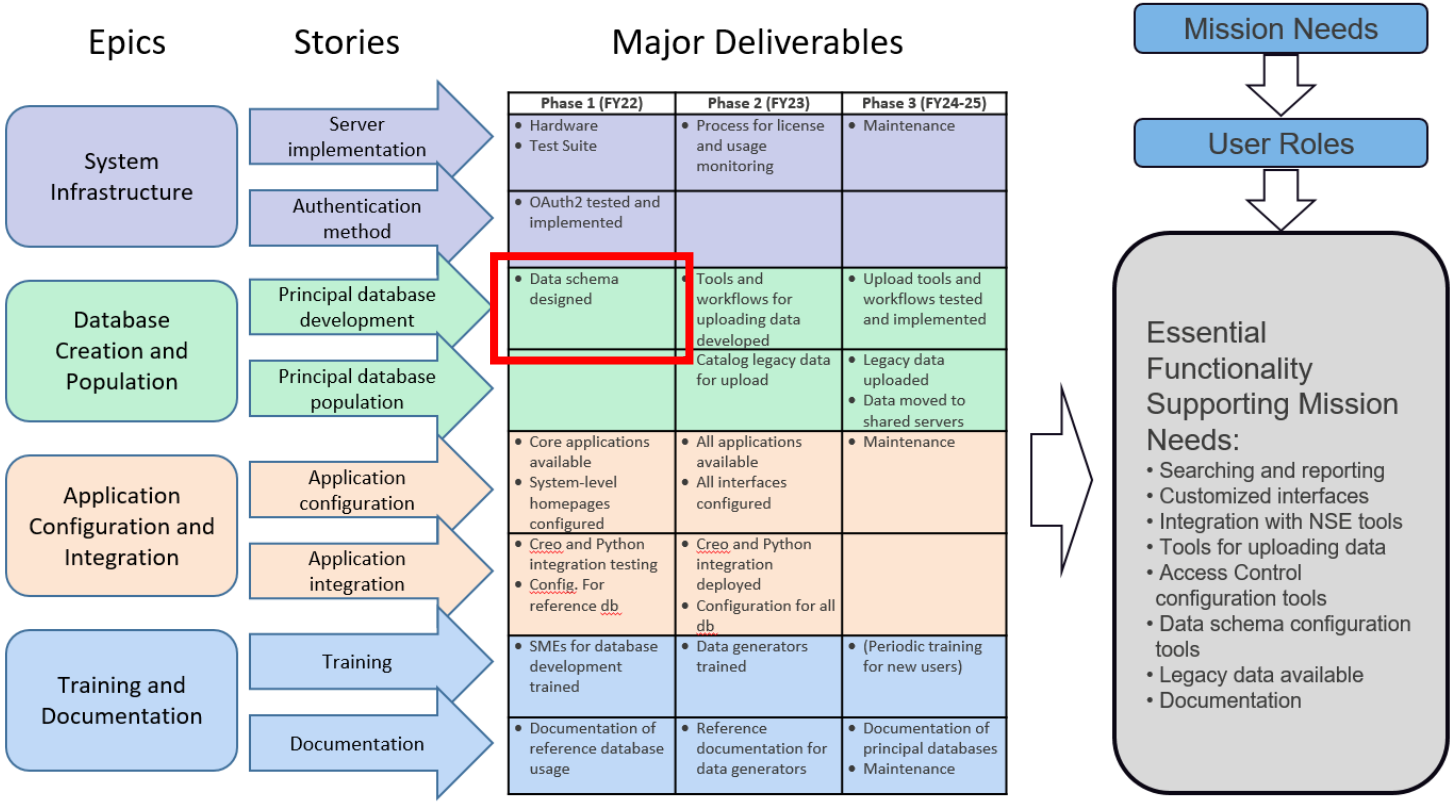
…45 types total

List of test data types and priority generated by cross-site collaboration

Configuration of Granta:MI for enterprise deployment needs support

- AMD (NA-115) supports LANL in this project
  - Funding is modest
  - Scope is confined to data types supporting AM
  - Progress is being made, but it is slow
  - Input from all sites is needed, but they have little (or no) funding
- Projects (e.g. At-Risk Materials, AM) continue to encourage Granta:MI use, *even without a standard schema*.
  - This will result in problems/limitations that will need to be resolved later
  - Better (quicker & cheaper) to standardize the schema *now*
- This project needs a home in NNSA

A notional plan for enterprise deployment was proposed to PRIDE in 2019, but only O&M falls within program scope

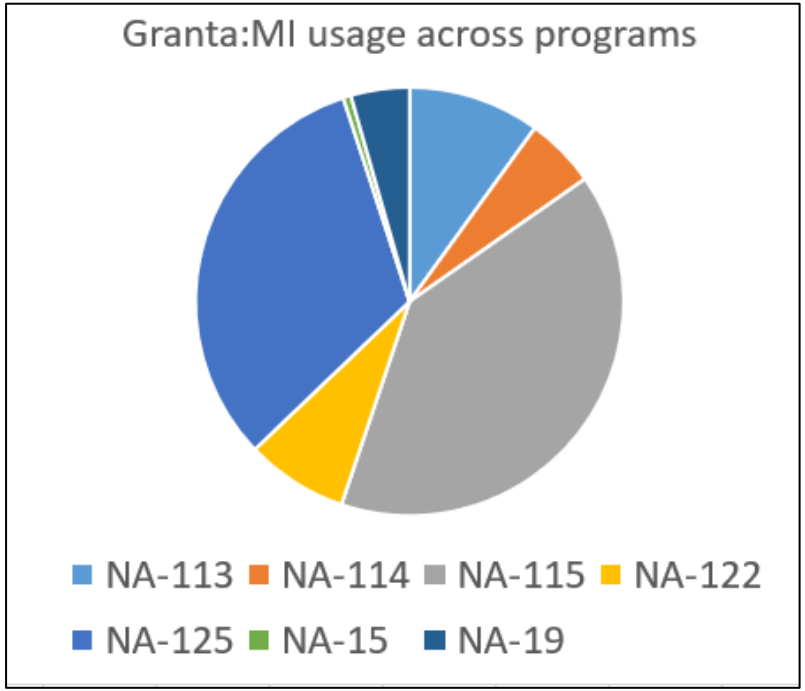


Thanks!
Questions, discussion?

Extra slides

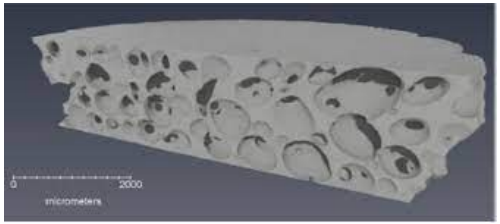
How much each program uses Granta:MI

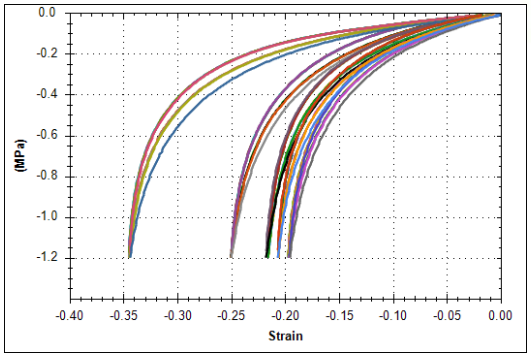
- Information on usage collected for FY20.
- NA-122.1 (PRIDE) requests programs split the ~$600k license cost according to usage.
- Individual projects assume the cost of uploading their own data.
  - Development and documentation funded by A&S minimizes these costs.



Types of tests performed by MST-7

- Mechanical
  - Uniaxial Compression & Tensile
  - Creep
- Thermal
  - Thermogravimetric Analysis (TGA)
  - Thermomechanical Analysis (TMA)
  - Differential Scanning Calorimetry (DSC)
  - Dynamic Mechanical Analysis (DMA)
- Imaging
  - Computed Tomography (CT)
  - Scanning Electron Microscopy (SEM)
- And more!





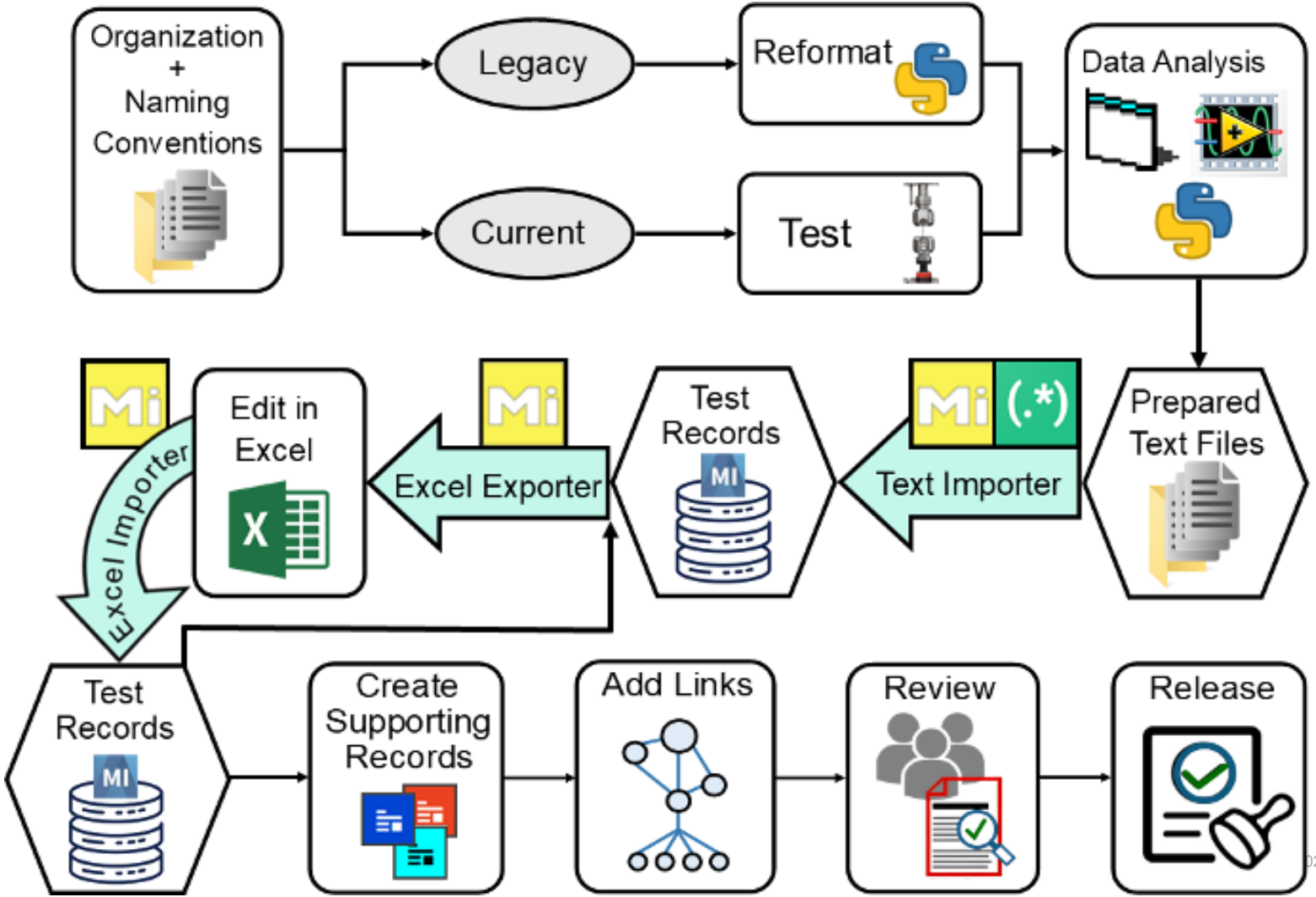
MST-7 Approach to Data Management

Need to overcome the paradigm of data/metadata living on individual hard drives, instrument computers, or in paper notebooks. No expectation to recall data/metadata after a project is finished.

- Establish a data management champion to help train and organize a team, as well as advocate to group management
- Capitalize on a robust student pipeline (cheap & not too busy yet)
  - Train to upload data to Granta, help develop uploading resources for busier test operators to use, set a new paradigm for data management in MST-7
- For new data: Incorporate data management into testing work packages
- For legacy data: Utilize students and A&S funding to gather, organize, and upload important, legacy weapons materials data

Lessons Learned

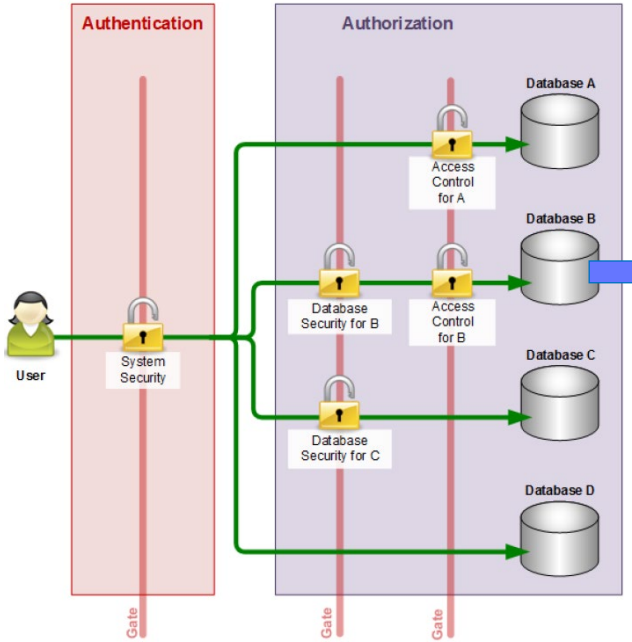
- **Standardization & Documentation is key!**
- Test programs that output standardized data files can be paired with a Granta importer
  - Students and myself put in the upfront effort to write test programs & importers for our common testing types (including as much metadata as possible)
  - Testing PIs are more willing to use our programs because of the paired importers
  - Importing becomes “1-click”
- Documenting the import & review processes helps distribute the workload and reduce onboarding effort of new PIs/students
  - Working on this in FY22 thanks to A&S funds


Organization + Naming Conventions
Legacy
Current
Reformat
Test
Data Analysis
Prepared Text Files
Text Importer
Test Records
Excel Exporter
Edit in Excel
Excel Importer
Test Records
Create Supporting Records
Add Links
Review
Release

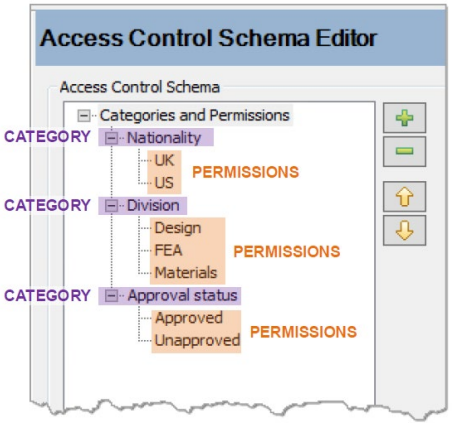
Lessons Learned

- There needed to be standard format for files associated with similar tests
- There needed to be guidance on how to name materials – we developed this
- Need other material properties such a density, modulus, sound speed, thermal conductivity. These were not usually documented.
- Older scientists were not using coding to automate processes – we changed that when I took over the project.
- Needed to develop schema for each different test – QS vs. SHPB or gas gun
- Iterate with import templates to improve the speed of uploading
- Need to assign tasks otherwise too overwhelming of a task
- Organize data even within our team to streamline uploading
- Sometimes we found the material and were able to do additional investigation to complete a dataset – microstructure information
- **Better to put in data right away than try to document 30 years later.**

Role-based permissions allow flexible access control



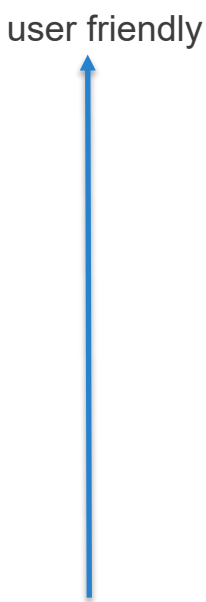
Fine-grained access control within each database



Example access control schema

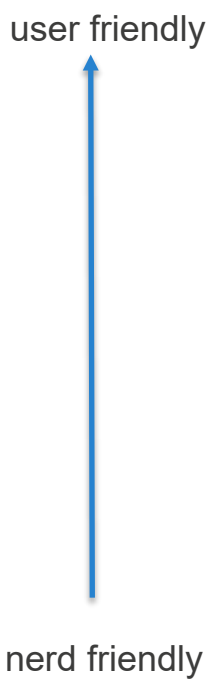
There are many ways to export data from the database.

- Printing record datasheets
- Export single records to Excel
- Export multiple records to Excel
- XML templates to export text files (e.g. in Abaqus keyword format)
- Python toolkit to retrieve data
- API to integrate data directly into other applications (e.g., Creo, Abaqus CAE, etc)



There are many ways to import data into the database.

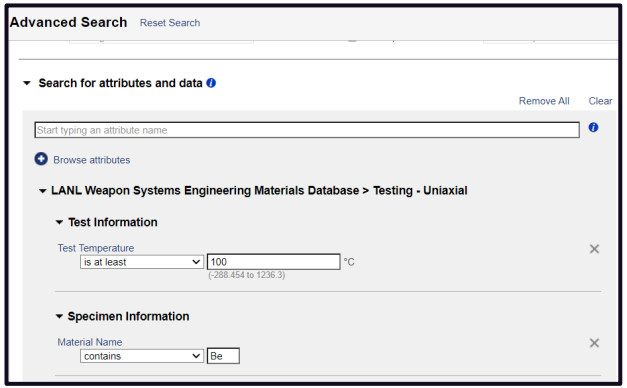
- Direct editing of records
- Excel templates to import single records
- Excel templates to import multiple records
- XML templates to import text files (e.g. output from test machines)
- Command line interface to facilitate scripting of large imports
- Python toolkit to import from user scripts



Consuming Granta data with MI:Viewer

- MI:Viewer contains useful but limited tools for searching, comparing, and exporting data

Search



Plot of results

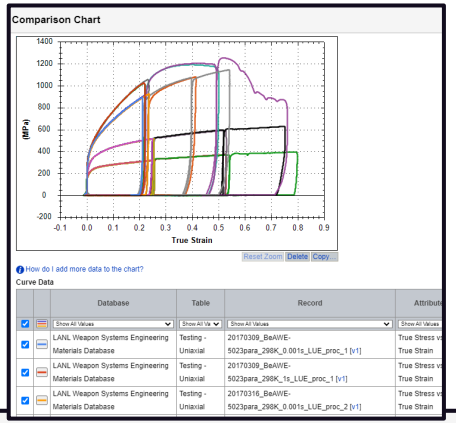
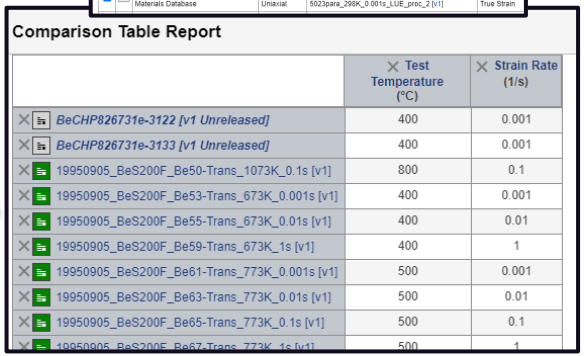
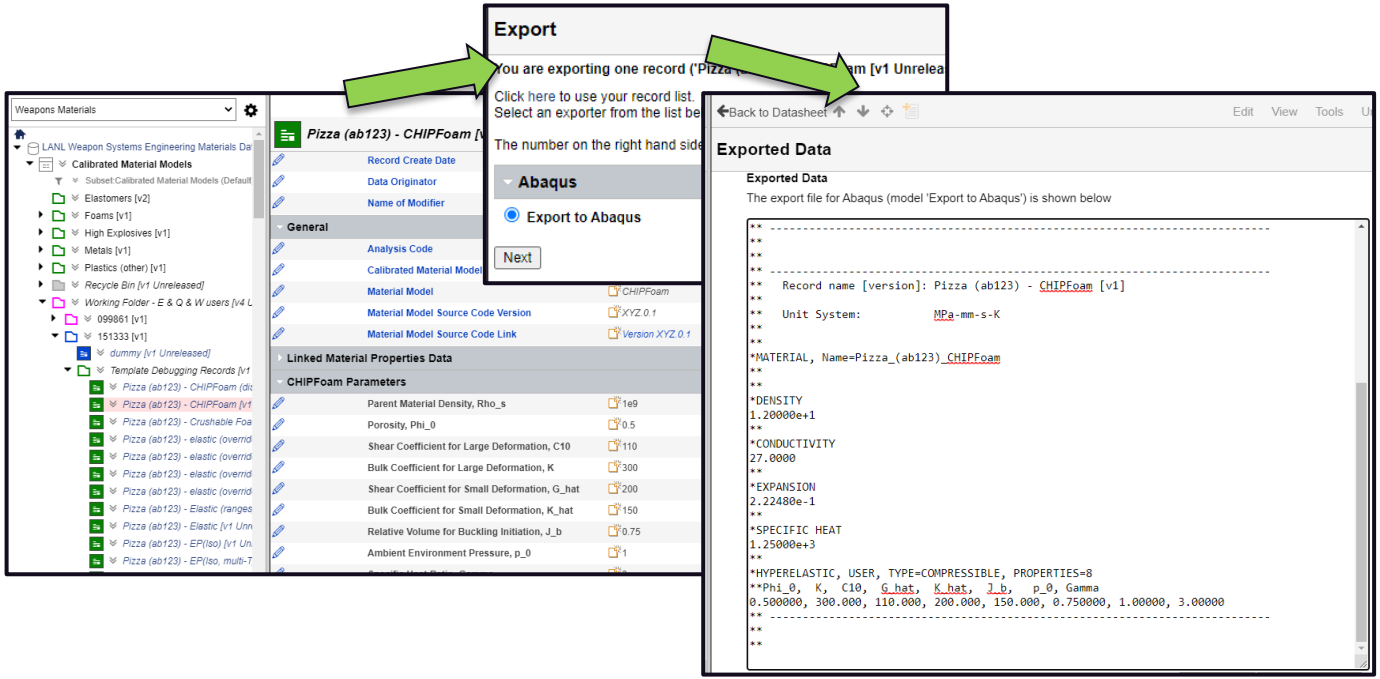


Table of results



Consuming Granta data with FEA exporters

- Material Model records can be exported (e.g. to Abaqus) using custom-configured xml export templates



Consuming Granta data with Gateways

- *MI Materials Gateway* connects Creo to Granta